

Towards a more complex description of chemical profiles in exoplanet retrievals: A 2-layer parameterisation

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## **Overview**

State of the art retrievals assume constant chemical profiles. In the context of next generation space telescopes (JWST [1] and Ariel [2]), this assumption may limit our ability to interpret exoplanets spectra. We implemented a "2-layer" retrieval parametrisation to independently extract molecular abundances above and below a certain atmospheric pressure. By comparing with the more traditional constant model, it showed that chemical assumptions have a significant impact on retrieved parameters (chemistry and temperature). From the simulation of cases inspired by real planets, we found that the 2-layer retrieval can successfully capture abundance discontinuities from disequilibrium processes and clouds/hazes.

**Ariel and JWST retrieval Methodology** For both JWST and Ariel, the retrieval is able to 0.0153 JWST simulation We add the 2-layer chemical module to the Fitted mode constrain the chemical abundances of an input 2-0.0152 bayesian retrieval suite TauREx [3]. layer model. 0.0151 Below are the spectra of a retrieval run for both 2-layer instruments on an HD 209458b like planet along 0.0150 The parametrisation requires 3 free parameters  $10^{-9}$ per molecules: with the posterior distribution for the JWST case. The surface abundant 0.0148 The input planet had an H2O 2-layer profile.



Figure 1: Example of a 2-layer chemical profile. The top mixing ratio here is 10<sup>-3</sup>, the surface mixing ratio is 5.10<sup>-10</sup> and the pressure separation occur at 10<sup>-3</sup> Bar.

- The top abundance
- The separation pressure

Then we simulate high resolution spectra using TauREx forward model. The observation is simulated by binning down using the JWST/Ariel response function [4][5]. Finally, TauREx retrieval mode is used to check whether the input parameters can be recovered.





Figure 2: Posterior distribution of the 2-layer JWST case.



Figure 3: Best fit spectra for an HD 209458 b like planet presenting a 2-layer chemistry. Top: JWST ; Bottom: Ariel.



## **Comparing 1-layer and 2-layer retrievals**

In order to compare the constant and the 2-layer models, we simulate a planet with a 2-layer chemical profile and perform the retrieval with the two models. In the investigated cases, the 2-layer retrieval performs well and is able to recover the input parameters. However, the retrieval using constant chemistry can present two issues:



Figure 4: Best fit Ariel spectra for the constant and 2-layer retrievals of a 2-layer H2O profile of an HD 209458 b planet.

- The observed spectrum cannot be explain using the 1-layer model and the best solution does not fit the data (not shown here)
- The 1-layer retrieval manages to get a 'good' fit, but the retrieved parameters are wrong (case presented in Figure 4 and 5 – see the retrieved temperature profile).

The first point is easy to spot due to the wrong fit. The second point is more subtle as there is no direct evidence of the mistake. Provided both retrievals are performed, statistical indicators such as the Nested Sampling Global Log-Evidence allow to break the problem as the 2-layer solution is clearly preferred (in this case log(E) = 906 for the 2-layer and log(E) = 744 for the 1-layer).

Figure 5: Chemical profiles (top) and temperature profiles (bottom) for the 2-layer and constant retrievals.

## **Examples of 2-layer chemistry**

The 2-layer approach can also be applied to real examples. We investigated the case of a Sub-neptune planet with photochemical hazes. The case is inspired from GJ 1214 b [6]. The input model investigated here involves:

- A Sub-Neptune size planet (0.216 MJ) with an Hydrogen-Helium envelope.

A decreasing temperature profile (3-point model) from 1300K to 700K.



- An H2O constant chemical abundance of 10<sup>-3</sup>.
- A CH4 decreasing 2-layer profile (10-3 for the surface and 10-6 for the top) corresponding to the condensation of hydrocarbons due to photochemistry.
- An upper atmosphere haze layer due to the photochemistry.

As seen on Figure 6 from the posterior distribution and the best fit model, it is possible to constrain an example of a planet with complex chemistry, temperature profile and cloud/hazes. In addition of providing valuable information on the chemical processes, the identification of condensation zone correlated with the apparition of hazes could help understanding their composition.

photochemical hazes resembling GJ 1214 b.

## References

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